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14. ABSTRACT
Wave propagation in the high frequency regime can be simplified using the geometrical optics approximation. We obtained an eikonal approximation for the phase and transport equations for the amplitude. The general strategy used to find the phase is to solve for its level sets, called wave fronts. This same strategy works to compute semiclassical solutions of Schrodinger's equation, which is the main topic we studied here. Traditional obstacles faced in numerical approaches are in dealing with multivaluedness and resolution of wave fronts. Under this contract we developed an Eulerian level set based method, solving for the wave fronts using both space and phase.

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Level Set Systems
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Level Set Systems (LSS) has done the following important research for AFOSR:

Wave propagation in the high frequency regime can be simplified using the geometrical optics approximation. We obtained an eikonal approximation for the phase and transport equations for the amplitude. The general strategy used to find the phase is to solve for its level sets, called wave fronts. This same strategy works to compute semiclassical solutions of Schrodinger's equation, which is the main topic we studied here.

Traditional obstacles faced in numerical approaches are in dealing with multivaluedness and resolution of wave fronts. Under this contract we developed an Eulerian level set based method, solving for the wave fronts using both space and phase. [JLOT1, JLOT2, CKOST, QCO, OCKST]

This approach immediately takes care of the issues of resolution and multivaluedness. However, memory becomes a nontrivial issue because of the high dimensionality of the problem which uses both physical and phase space. This difficulty was fixed using a novel fast growing algorithm for geometrical optics in [Ch]. It was based on an original seeding design and an efficient, high order accurate semi-Lagrangian method for solving Liouville equations. We can now solve 6 dimensional problems on a 200^6 uniform mesh. Moreover, in [JW], effective Hamiltonian preserving schemes for the Liouville equation with partial transmissions and reflections were devised. This is needed for problems with discontinuous indices of refraction.

However, to compute amplitudes accurately through caustics using this approach, we need to identify the caustics and use the Keller-Maslov index to continue through them. A very promising new approach to this problem involves the use of Gaussian beams [TQR, Ra]. As part of this work statement we have used Gaussian beams to compute high frequency solutions of Schrodinger's equation, which arises in QVNE: quantum vacuum nanoelectronics.

These beams are approximate solutions of hyperbolic partial differential that are

concentrated on a curve in space-time. They have an adaptive property so that even a Lagrangian approach appears to be superior to straightforward ray tracing because a) the asymptotic solution is valid through caustics so there is no need to identify the caustics beforehand, and b) only the superposition of a few beams is needed to accurately compute an entire wave front for moderate times, without using interpolation.

In addition to pursuing this Lagrangian approach for QVNE (which is, of course, a bit more complicated than standard ray tracing) we have investigated a semi-Lagrangian level set approach [LQO] with very encouraging results.

We have earlier [JLOT2] applied the level set Liouville approach to the semiclassical method for quantum mechanics. We begin with the Schrödinger equation:

(1)
$$\begin{aligned} i\hbar\,\psi_t &= \frac{\hbar^2}{2m}\Delta\psi + \nu(x)\psi \\ \psi(x,0) &= \psi_0(x) \end{aligned}$$

Where $\psi(x,t)$ is the wave function; $\nu(x)$ is the potential. Resolving oscillations of wavelength $\hbar$ is impossible with modern (and foreseeable) computers.

Alternatively we used semiclassical methods which link classical mechanics to quantum mechanics. .

(I)We extended our Eulerian /level set techniques and results in [JLOT2], extending the semi-Lagrangian approach of [Ch] to compute the phase S which satisfies

(2)
$$S_t + \frac{|\nabla S|^2}{2} + \nu(x) = 0, \quad S(0,x) = S_0(x)$$

Of course, the issue of computing amplitudes through caustics again arises here.

(II)We used Gaussian Beams to deal with the issue of caustics [TQR, Ra]. Again, the superposition enables us to continue through caustics and get an effective semiclassical approximation. The canonical system consists of equation (2) for the phase and

(3)
$$\frac{\partial\varphi}{\partial t} + \nabla S\cdot\nabla\varphi + \frac{1}{2}(\Delta S)\varphi = 0, \quad \varphi(x,0) = \varphi_0(x)$$

for the amplitude.

We modify the integral data S_0 to have a positive imaginary part centered at some initial point.

We arrive at a Hamiltonian system (as in ray tracing) but we also needed to

solve matrix valued ODE's.

We extended the Gaussian beam summation method for solving Helmholtz' equations in the high frequency regime. The traditional Gaussian beam summation method is based on Lagrangian ray tracing and local ray-centered coordinates. In [LQB] a new Eulerian formulation of Gaussian beam theory was developed. This yields uniformly distributed Eulerian traveltimes and amplitudes in phase space simultaneously for multiple sources. Time harmonic wavefields can be constructed by summing up Gaussian beams in the new Eulerian formulation. Lagrangian Gaussian beam summation can be derived from this method.

The advantages of this new method are: (1) Uniform resolution of ray distribution. (2) We can obtain wavefields excited at different sources by varying only source locations in the summation formula. (3) We can obtain wavefields excited at different frequencies by varying only frequencies in the summation formula. Thus we seem to have constructed a viable Eulerian alternative to ray tracing. This should be of use to the Air Force.

There are many applications of interest to the Air Force. Nano devices are always useful. As microelectronics becomes nanoelectronics new numerical approaches are needed in order to deal with the quantum scale. We believe our methods developed here are appropriate for this challenge.

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